

Isonipecotinoylisonipecotic acid, N'-(4-fluoro-2-trifluoromethylbenzoyl)-, ethyl ester

InChI: InChI=1S/C22H26F4N2O4/c1-2-32-21(31)15-7-11-27(12-8-15)19(29)14-5-9-28(10-6-14)30
InChIKey: XXVZIPITMNFJRZ-UHFFFAOYSA-N

Formula: C22H26F4N2O4

SMILES: CCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3ccc(F)cc3C(F)(F)F)CC2)CC1

Mol. weight [g/mol]: 458.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.498		Crippen Method
mcvol	312.980	ml/mol	McGowan Method
rinpol	3232.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361259&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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